Impact of Dispersion of gases from combustion of Coal tar

Dissertation Submitted

To

The department of Chemical Engineering

Of

National Institute of Technology, Rourkela

In partial fulfillment of the requirements

For the degree of

Bachelor in Technology

By

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Certificate

This is to certify that the work in the thesis entitled *Impact of Dispersion of gases from combustion of Coal Tar, by V Divya Sree* bearing roll number *111Ch0425* is a record of an original thesis work carried out by her under my supervision and guidance in partial fulfillments of the requirements for the award of degree of Bachelor of Technology in Chemical Engineering

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Assistant Professor,

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Declaration

I hereby declare that all the work contained in this report is my own work unless otherwise acknowledged. Also, all of my work has not been previously submitted for any academic degree. All sources of quoted information have been acknowledged by means of appropriate references

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Acknowledgement

I would like to express my deepest gratitude to the people who helped me with the work presented in this dissertation, be it through supplying alternative and usually simplifying views during scientific discussions, or through moral support during periods of stress and doubt, or by providing the possibility of embarking on the extraordinary experience of participating in this adventure.

Firstly, I am deeply indebted to my supervisor**, Dr. Basudeb Munshi**. He provided an open and free environment that allowed me to choose this topic and provided valuable insight that helped me in completing the project. I would also like to acknowledge his exemplary guidance, monitoring and constant encouragement throughout the course of this thesis.

I present many thanks to all my professors who over the years have molded me in the field of Chemical Engineering. I would like to convey my special regards to Mr. Akhilesh Sir for helping me with the rapid software without whom this project would be almost incomplete.

I am very much thankful to those, who have been giving inspiration and kind advice without which, it would not have been possible for me to complete this project work .I thank all my friends and well-wishers who have rendered help in this endeavor.

ABSTRACT

This project 'Impact of Dispersion of gases from combustion of Coal tar' deals with gases released during combustion of Coal tar and the area affected by these gases. This depends on many parameters. This is solved by using the software "ANSYS". For modeling, the parameters which affect the flow of gases are need to be known. In general, wind flow, presence of obstacles and temperature may affect the flow.

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1. INTRODUCTION

1.1 Coal tar

Coal tar is a brown or black liquid of extremely high viscosity. It is among the byproducts when coal is carbonized to make coke. This is mixture of Phenols, polycyclic aromatic hydrocarbons and heterocyclic compounds. The composition of coal tar is influenced by the origin and composition of coal and also by the nature of distilling process. As a result, it is referred by many names coal tar, crude coal tar, coal tar pitch, coal tar creosote.

Combustion of coal tar is burning coal tar in presence of oxygen .The gases released are Sulphur dioxide, carbon monoxide, carbon dioxide, NOx. Some particulates are also released like ash.

1.2 Chemical composition (%)

Carbon	92-93
Hydrogen	4.3-4.7
Sulphur	0.3-0.8
Nitrogen	1.7-1.8
Oxygen	0.8-1
Ash content	0.2-0.3

Density 1.2-1.3gm/cm3

2. LITERATURE REVIEW

This chapter summarizes all the back ground reading done to gain enough knowledge of software Ansys, parameters affecting the flow of cloud.

2.1 ANSYS

Ansys is an Engineering simulation software. Out of the different programs present, ANSYSCFD is mostly used. ANSYS CFD is used in systems by simulating fluid Flows in a virtual environment. This is mostly used in aircraft hydrodynamics, hydro cyclones etc.

The present project work utilizes ANSYS 15.0 where Workbench is used for the geometry purpose while the further simulation is done using Fluent 6.2.16. The mass fraction of different gases and pressure profiles are observed at different velocities of the wind and at different velocities of the gases coming out. The mass fraction for different gases at different distances along the horizontally and as well as vertically are obtained and are checked with ambient conditions.

2.2 PARAMETERS AFFECTING THE FLOW

The gases released generally form a cloud and move. At low concentrations all the gases are transported and dispersed through the atmosphere in the same way. The internal cloud buoyancy is the measure of whether the in cloud density is greater than or less than the ambient or environmental density. If the cloud density is greater than ambient density, it is called dense. If it is less dense, then it is called buoyant, and it may rise several hundred meters away

The turbulent dispersion(i.e. rate of speed in lateral ,vertical ,downward direction)of the cloud about its center of mass depends on atmospheric turbulence in the atmosphere which itself depends on surface roughness conditions, the wind speed, and stability(i.e. day or night).because of this the geographic area covered by the cloud will increase ,thus affecting larger population .Buoyant turbulence is generated by heating of the ground surface by the sun and its suppressed by cooling of the ground surface at night.

Urban heat-Because of heat generated by human activities, including industrial processes, urban or industrial areas is often several degrees warmer than its surroundings. This causes the cloud to be neutral or unstable.

Aerosols and particles with sizes greater than about 10micrometer will have appreciable settling velocities. For e.g., cloud of 200 micrometer aerosols released near the ground will settle to the ground in a few minutes. Particles less than 10 micrometer have velocities so small that they remain suspended.

2.4 SUMMARY OF REVIEW

This chapter has gone over all the concepts vital to this project in detail. It has covered all the background knowledge in the field of dispersion of gases that is necessary for the simulation.

3. MODELLING AND SIMULATION

3.1 THE PROBLEM STATEMENT

The present project work consists of 3D rectangular area having horizontal distance of1000m, vertical distance of 3500m and width of 500m. Inside the rectangular area coal tar is combusted at a temperature of 500k, in an area of 5*5 m at a distance of 50 m from the flow of wind. Wind is flowing in positive X-direction and considering the different velocities of wind as 1m/s, 3m/s, 5m/s, 7m/s,9m/s,11m/s,13m/s,15m/s,17m/s,19m/s. velocities of gases are taken as 1 m/s. Mass fractions of the pollutants (SO_2, NO_2, CO, PPM_{10}) coming out are known. Mass diffusivities of different pollutants with respect to air are also known. For a constant value of gases velocity by varying the wind velocity, different types of dispersion is observed. The geometry of the problem is created using Workbench, followed by meshing. The rest of work which includes providing initial and boundary conditions etc. is done in Fluent. Thus the concentration of pollutants at different heights and horizontal distance is calculated using ANSYS. Tabulation and plotting is done to get an idea about the relation among the pollutants concentration and distance.

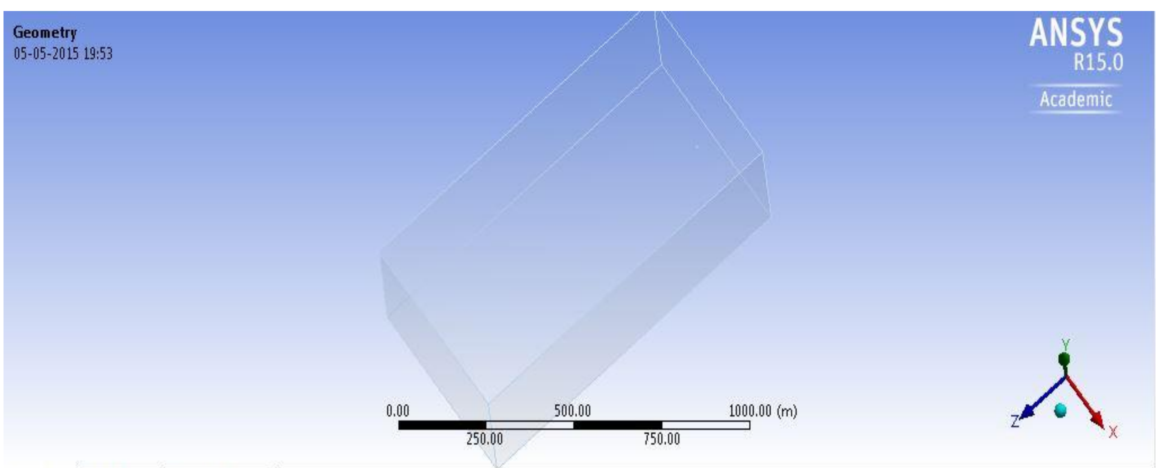

Figure 3.1 Geometry of the physical domain with length 1000m, breadth 500 and width 500m

Emissions of Pollutants (Mass fractions)

SO_2- 0.003

NO_x- 0.017

CO- 0.058

CO_2- 0.92

3.2 MESH

Meshing is basic requirement for the simulation process. To analyse the fluid flow problems, the flow domains are divided into the smaller subdomains. For the meshing, fine tetrahedron mesh is done in 3d geometry. After that named selection was done which was named as inlet, inlet1, symmetry, wall for the entire geometry.

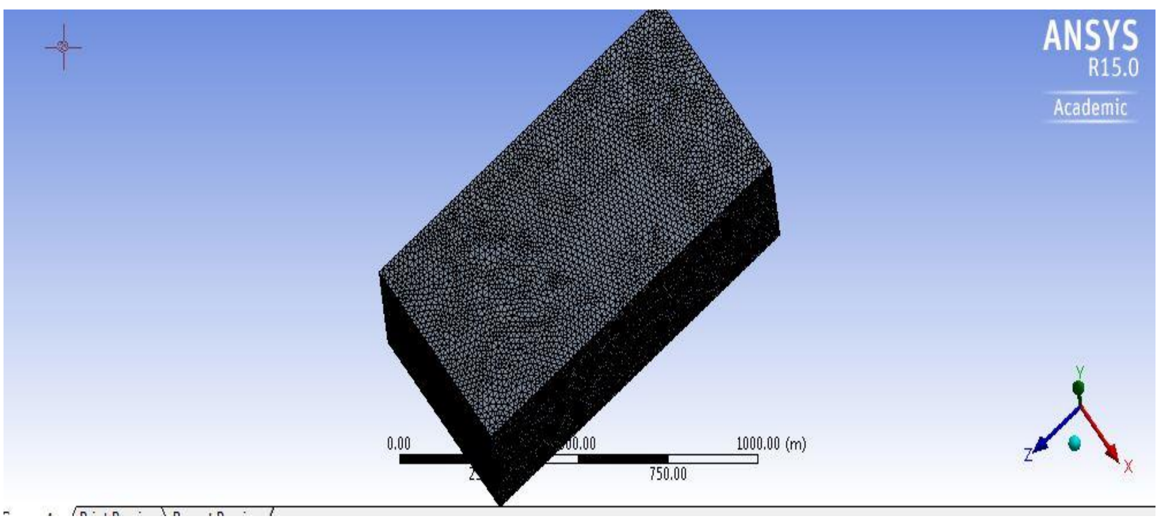

Figure 3.2 Meshed Geometry of the physical domain

3.3 MODELLING EQUATIONS

3.3.1 Continuity equation

Equation for mass conservation equation or also known as continuity equation is written as:-

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \overline{v}) = S_m$$

3.3.1

3.3.2 Transport equation for species transport

For the species transport in ANSYS FLUENT it solves the transport equation inside the domain which is given as :-

$$\frac{\partial \alpha_l \rho_l \phi_l^k}{\partial t} + \nabla \cdot \left(\alpha_l \rho_l \overline{u}_l \phi_l^k - \alpha_l \Gamma_l^k \nabla \phi_l^k \right) = S_l^k \quad k = 1, \ldots, N$$

3.3.2

3.4 SOLUTION METHODOLOGY

For the simulation process Phase coupled SIMPLE was chosen for the pressure-velocity coupling. Second order Upwind scheme was chosen for the discretization of partial differential equation. In the final step of simulation iterations were given which were as follows:-

Step size – 0.05

Number of steps – 10000

4. Effect of Wind Velocity on the Dispersion of Gases

4.1 Wind velocity of 1m/s

4.1.1 Dispersion of SO_2

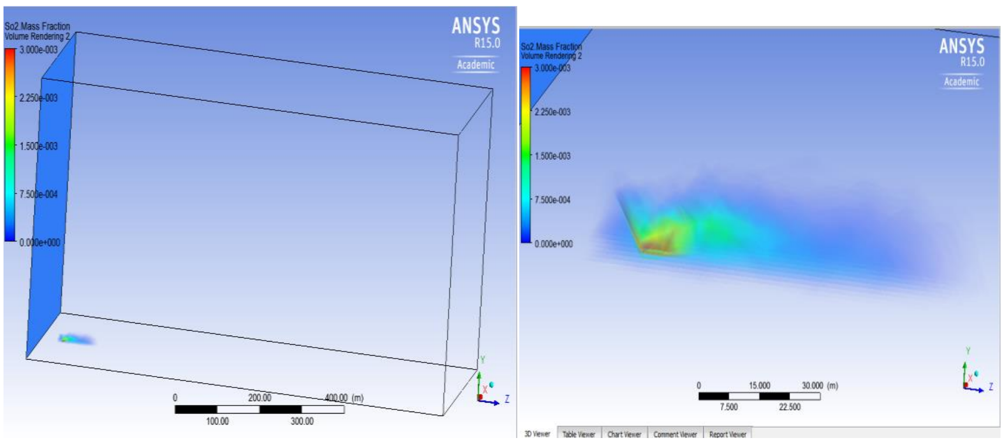

Figure 4.1.1 Dispersion ofSulphur dioxide

Contour clearly shows the dispersion of Sulphur dioxide gas .The dispersion is very less.

4.1.2 Dispersion ofNO_x

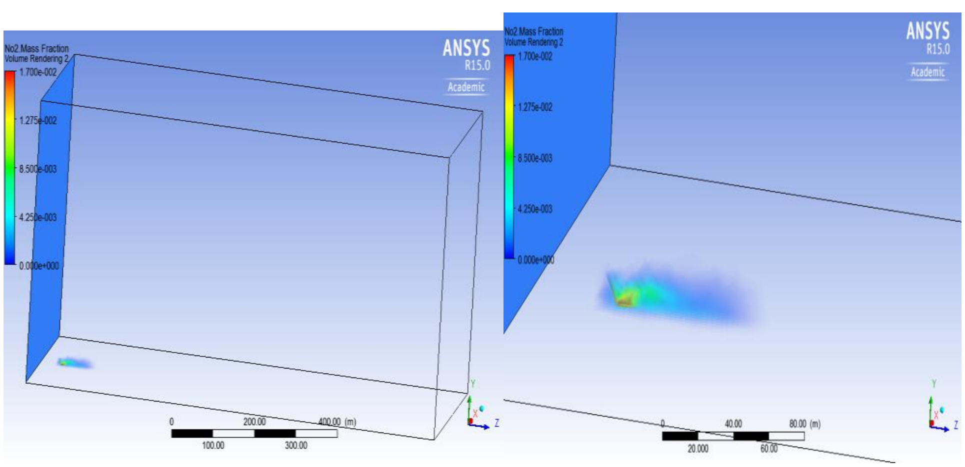

Figure 4.1.2 Dispersion of Nitrogen oxide

Contour clearly shows the dispersion of nitrogen oxide gas .The downstream length covered by the gas is less.

4.1.3 Dispersion of CO

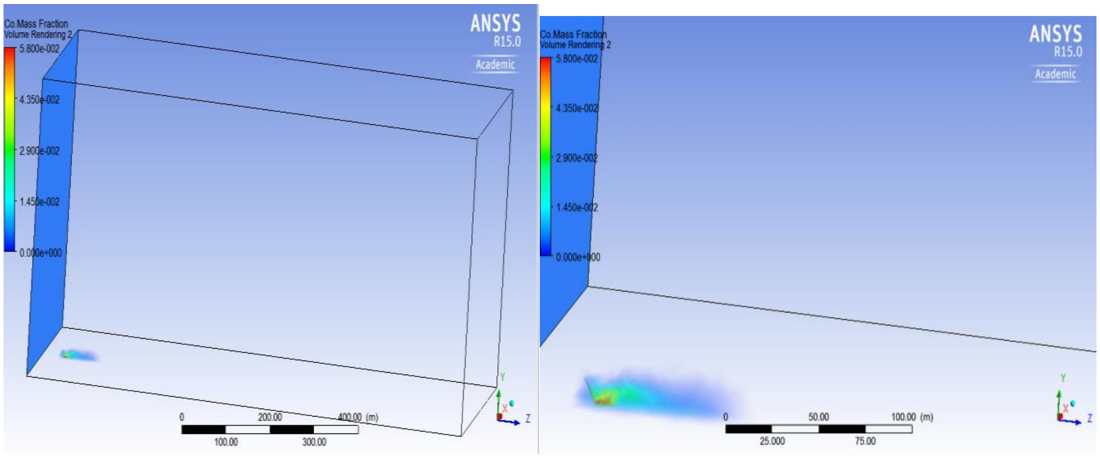

Figure 4.1.3 Dispersion of Carbon monoxide

Contour clearly shows the dispersion of carbon monoxide gas.Dispersion is very less and the mass fraction is maximum near the combusted area and it decreased in downstream length.

4.1.4 Dispersion of CO_2

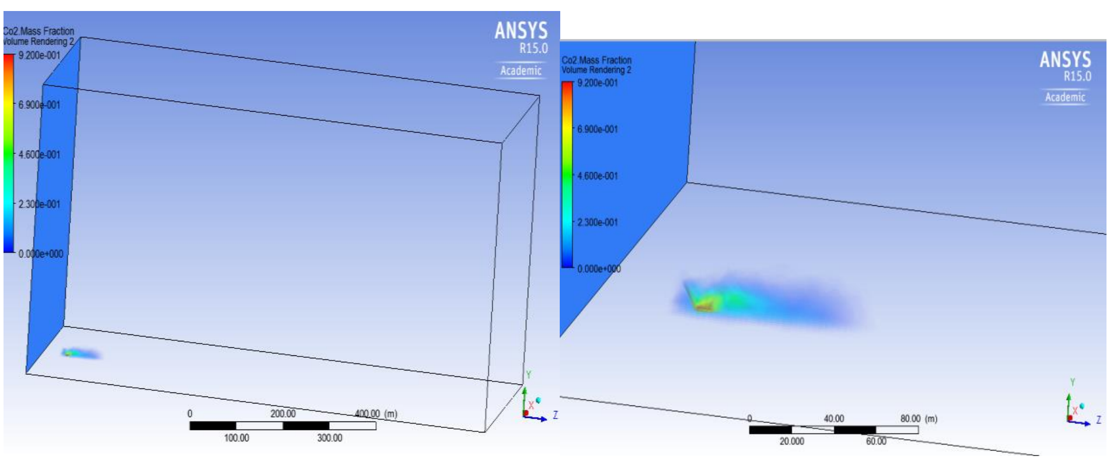

Figure 4.1.4 Dispersion of Carbon dioxide

The extent of dispersion is less and the mass fraction is maximum near the area where coal is combusted and it is reduced in the downstream length.

4.2 Wind velocity of 19m/s

4.2.1 Dispersion of SO_2

The contour clearly shows the dispersion and it is very clear that the downstream length to which the gas had been dispersed is more than that compared to the length covered by gas at 1m/s.

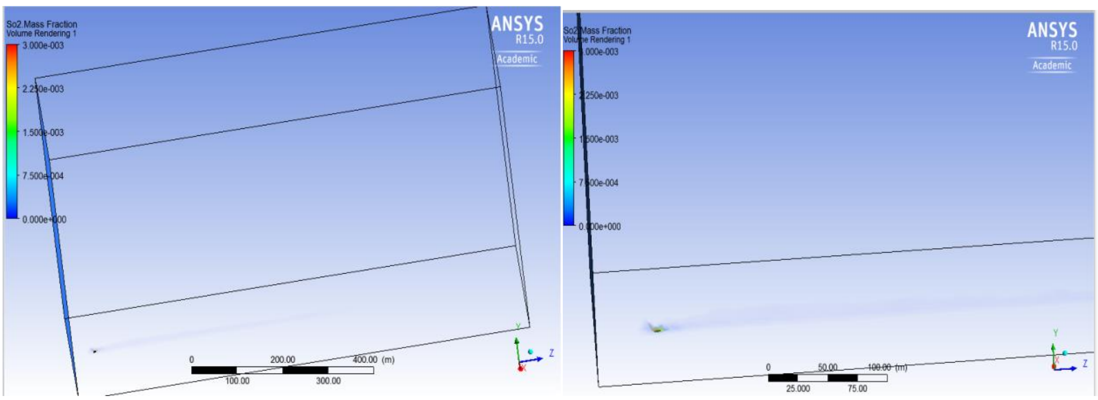

Figure 4.2.1 Dispersion of Sulphur dioxide

4.2.2 Dispersion of NOx

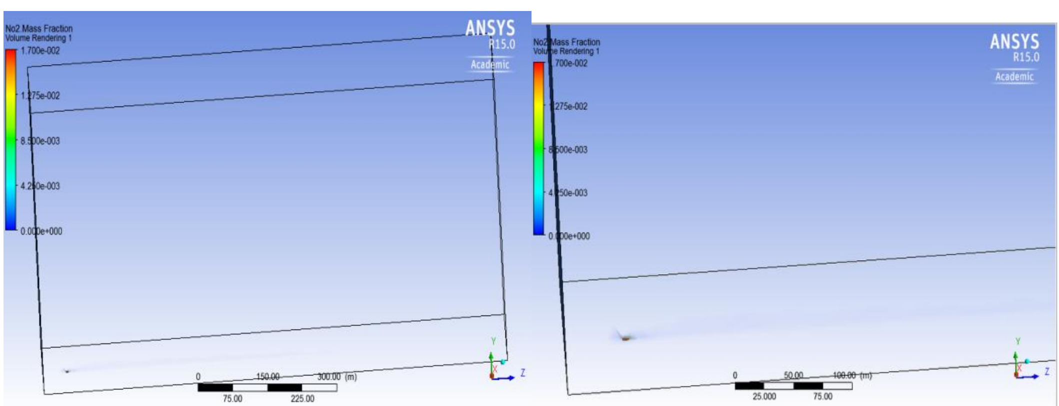

Figure 4.2.2 Dispersion of Nitrogen oxide

The dispersion is high in this case as compared to that of wind velocity at 1m/s.

4.2.3 Dispersion of CO

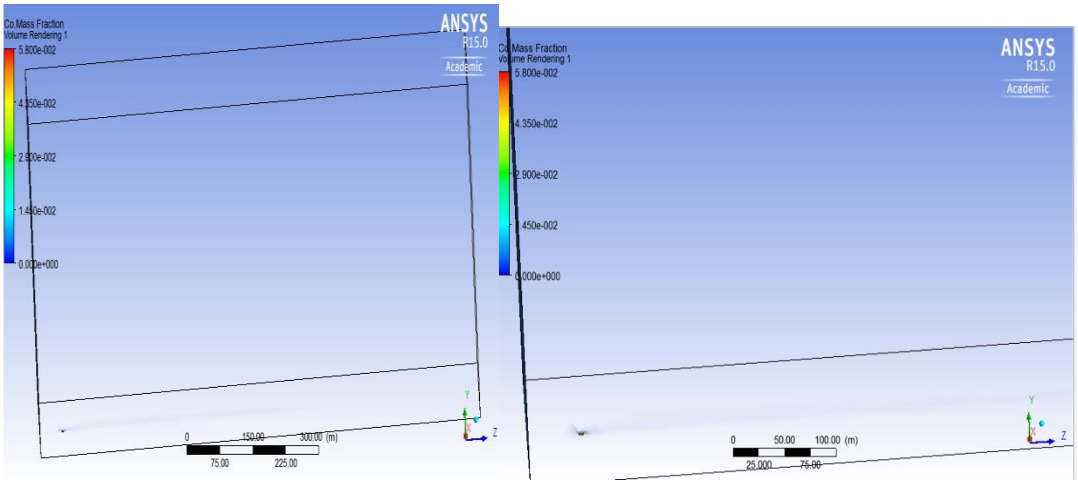

Figure 4.2.3 Dispersion of Carbon monoxide

The contour clearly shows the dispersion and it is very clear that the downstream length to which the gas had been dispersed is more than that compared to the length covered by gas at 1m/s.

4.2.4 Dispersion of CO_2

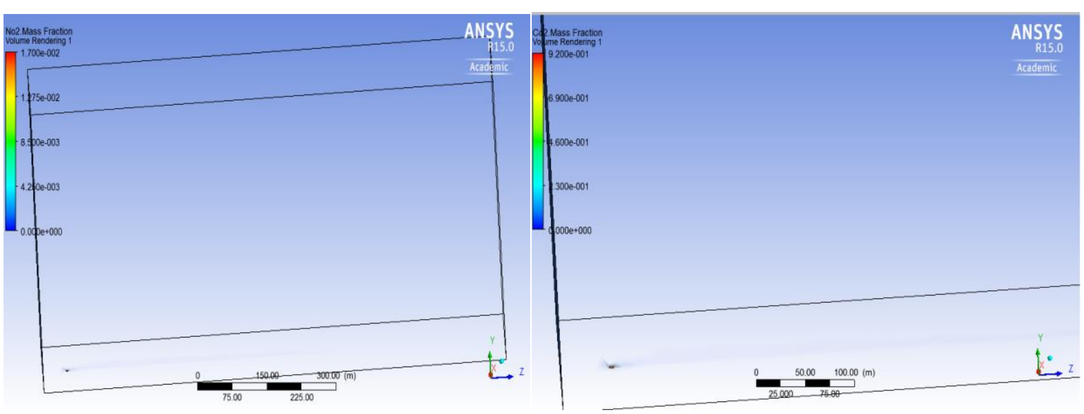

Figure 4.2.4 Dispersion of Carbon Dioxide

The dispersion is high in this case as compared to that of wind velocity at 1m/s.Mass fraction is decreasing in the downstream.

5. RESULTS & DISCUSSION

Level 1 is taken as ground level .Level 2 is at a distance of 4m from ground level. Level 3 is taken at a distance of 8m from ground level. Level 4 is taken at a distance of 12m from ground level. Level 5 is taken at a distance of 16m from ground level. Level 6 is taken at a distance of 25m from ground level.

5.1 Wind velocity at 1m/s

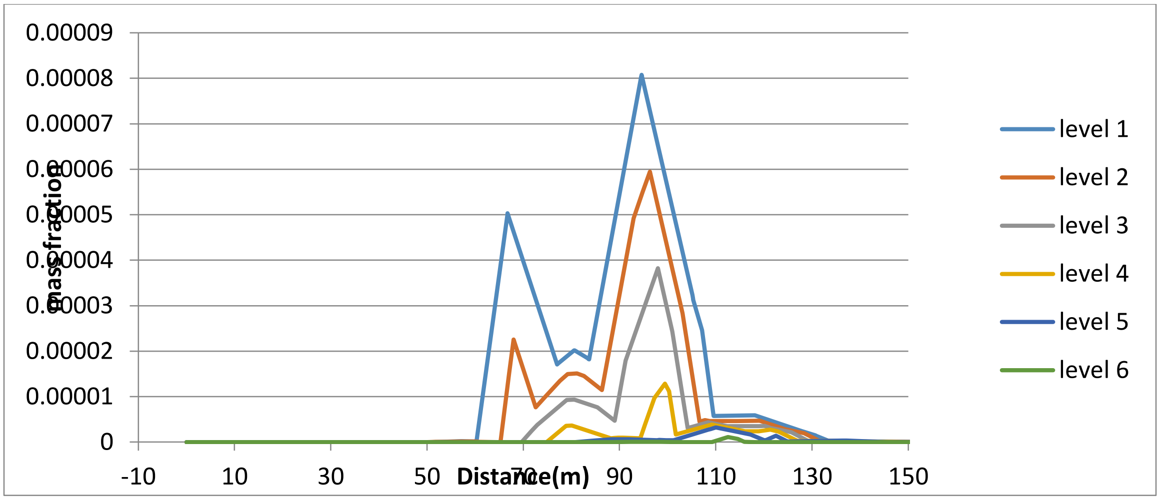

Figure 5.1.1 Sulphur dioxide dispersion

SO_2gas is following a particular trend when the inlet velocity is 1m/s at all the levels. The downstream length affected by the gas is 130m and the maximum mass fraction is present on ground at a distance of 100m.

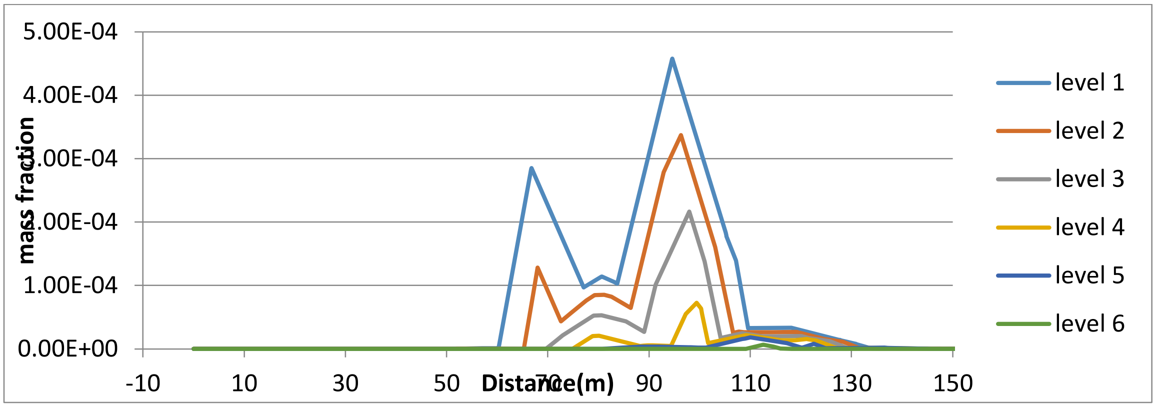

Figure 5.1.2 NO_x dispersion

NOx gas is following a particular trend at all levels and the downstream length affected by the gas is 130m and the maximum mass fraction is 0.00045 on ground is at a distance of 100m.The concentration of the gas has been decreasing from level 1 to level 6 and maximum concentration is at level 1.

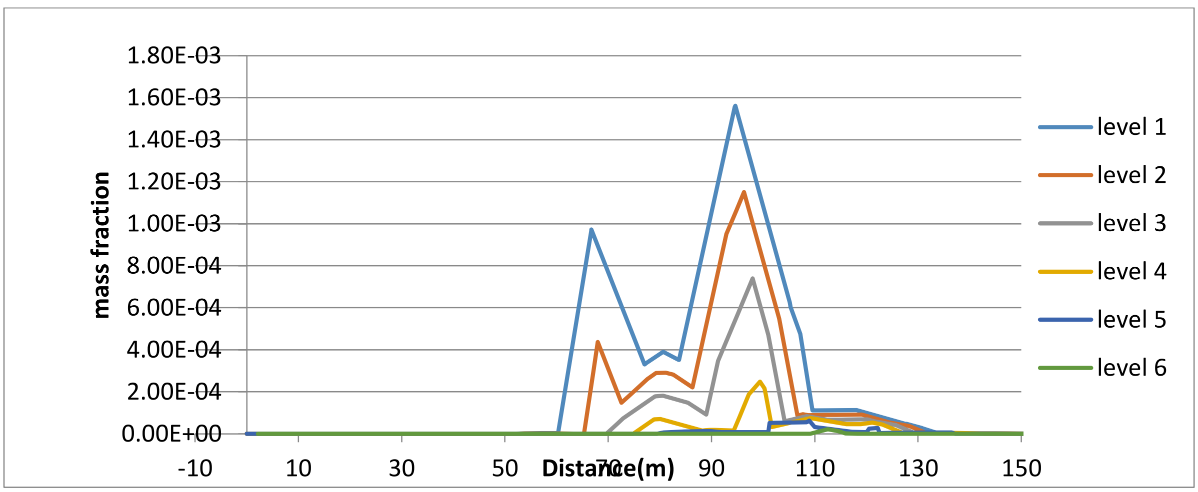

Figure 5.1.3 Carbon monoxide dispersion

CO gas is following a particular trend at all levels and the downstream length affected by the gas is 130m and the maximum mass fraction is 0.0016 on ground is at a distance of 95m.At 25m height the concentration of gas has become zero.

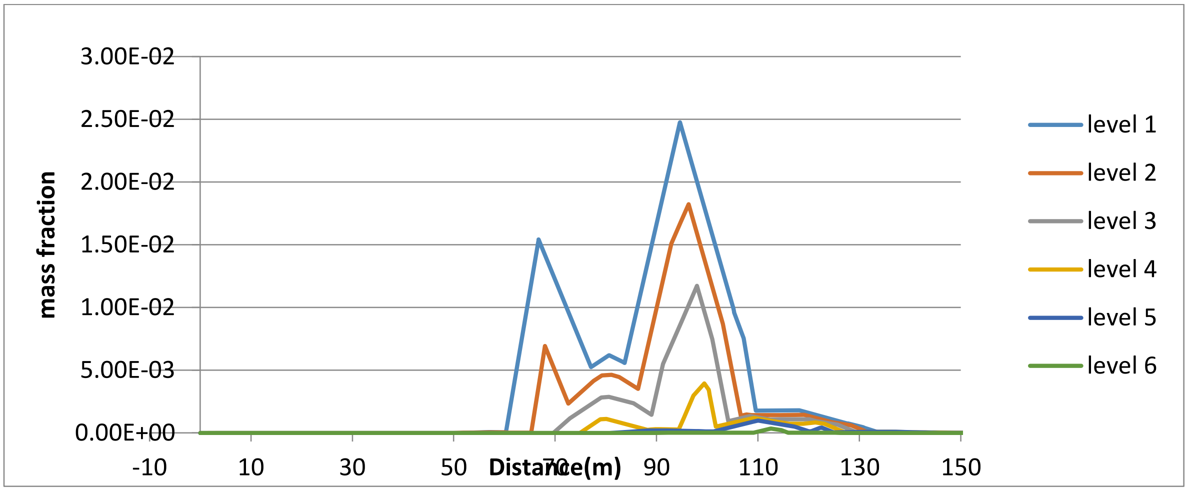

Figure 5.1.4 Carbon dioxide dispersion

CO_2 gas is following a particular trend at all levels and the downstream length affected by the gas is 140m and the maximum mass fraction is 0.025 on ground is at a distance of 97m.The concentration of the gas has been decreasing from level 1 to level 6 and maximum concentration is at level 1.

5.2 Wind velocity at 3m/s

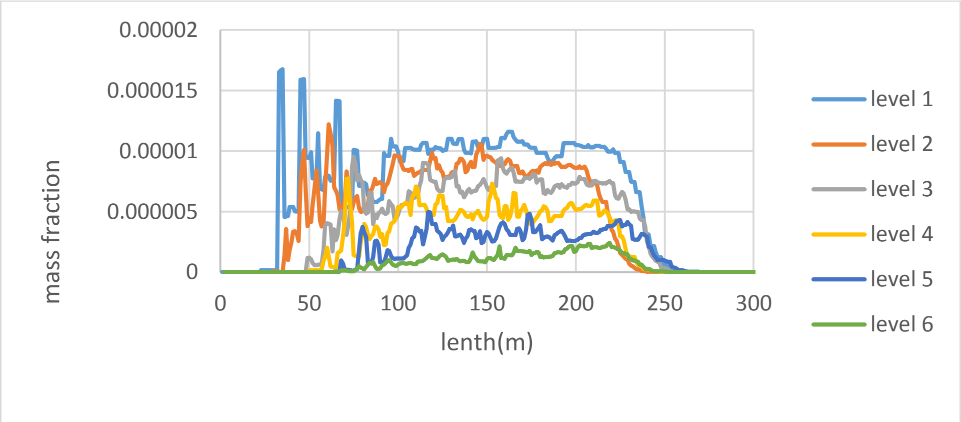

Figure 5.2.1 Sulphur dioxide dispersion

SO_2 gas had moved 270m downstream distance and the maximum mass fraction is 0.000017 on ground and the concentration has been decreasing as the height has been increasing.

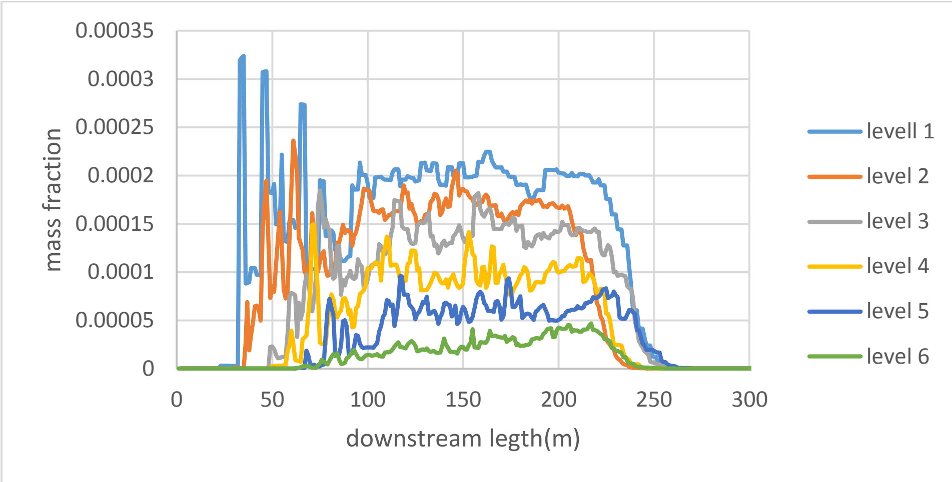

Figure 5.2.2 Carbon dioxide dispersion

CO_2 gas had moved 260m downstream distance and the maximum mass fraction is 0.00032 on ground and the concentration has been decreasing as the height has been increasing. The distance covered by the gas has increased as we increased the velocity.

5.3 Wind velocity at 5m/s

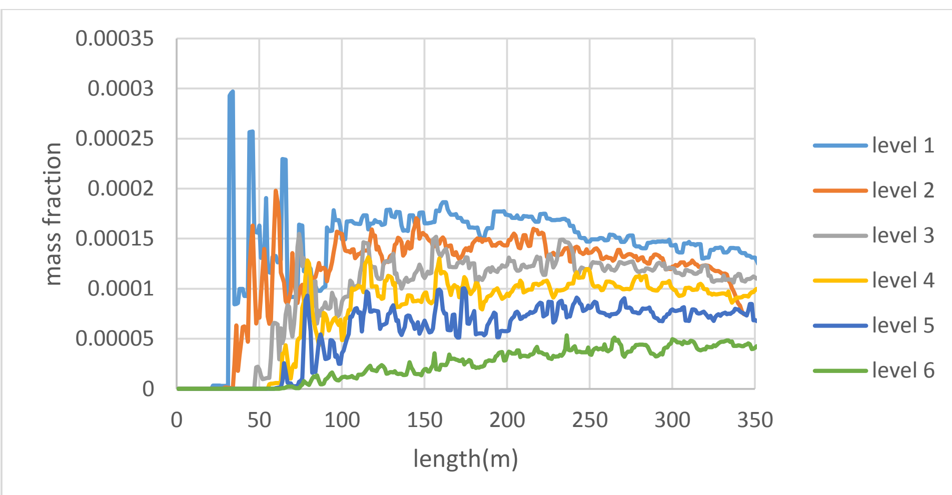

Figure 5.3.1 Carbon monoxide dispersion

CO gas had moved 350m downstream distance and the maximum mass fraction is 0.0003 on ground and the concentration has been decreasing as the height has been increasing and also in the downstream distance.

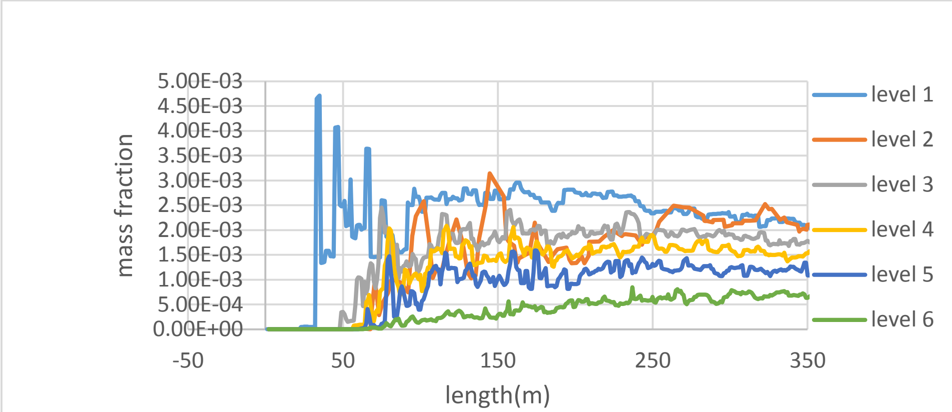

Figure 5.3.2 Carbon dioxide dispersion

CO_2 gas had moved 360m downstream distance and the maximum mass fraction is 0.0049 on ground and the concentration has been decreasing as the height has been increasing. The distance covered by the gas has increased as we increased the velocity.

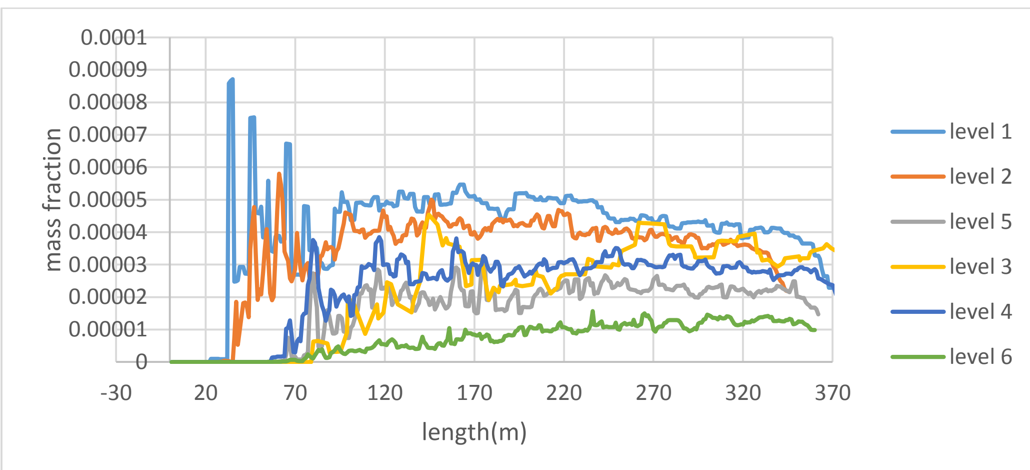

Figure 5.3.3 Nitrogen oxide dispersion

NOx gas had moved 370m downstream distance and the maximum mass fraction is 0.00009 on ground and the concentration has been decreasing as the height has been increasing and the concentration at level 6 is minimum which is nearly 0.00001.

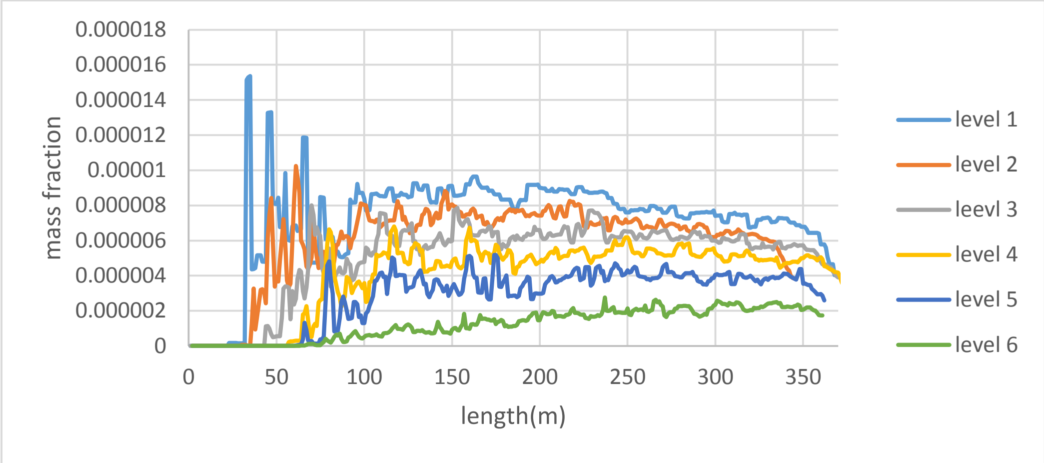

Figure 5.3.4 Sulphur dioxide dispersion

SO_2 gas had moved 370m downstream distance and the maximum mass fraction is 0.000015 on ground and the concentration at level 6 is minimum which is nearly 0.000002.

5.4 Wind velocity at 7m/s

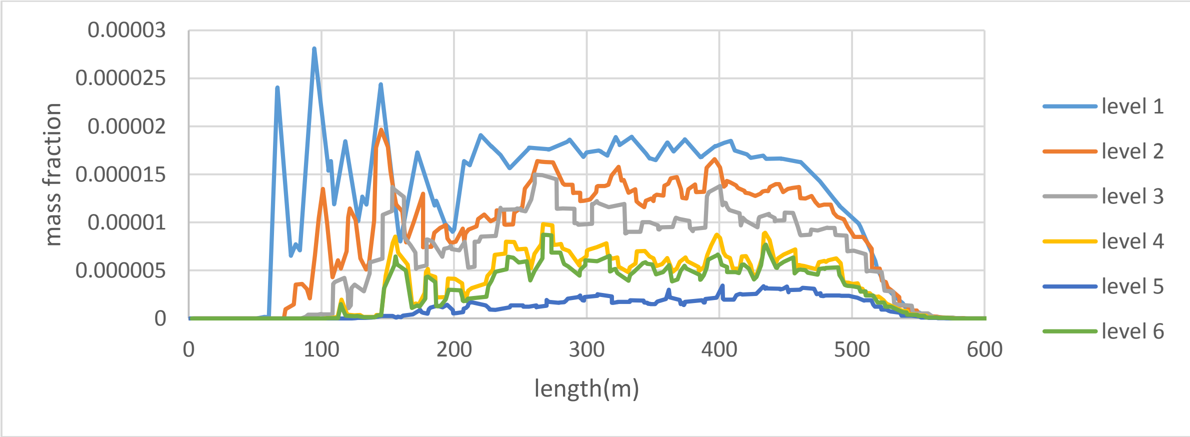

Figure 5.4.1 Sulphur dioxide dispersion

SO_2 gas covered a distance of 550m and the maximum mass fraction is 0.000027 on the ground and the concentration is decreasing downstream.

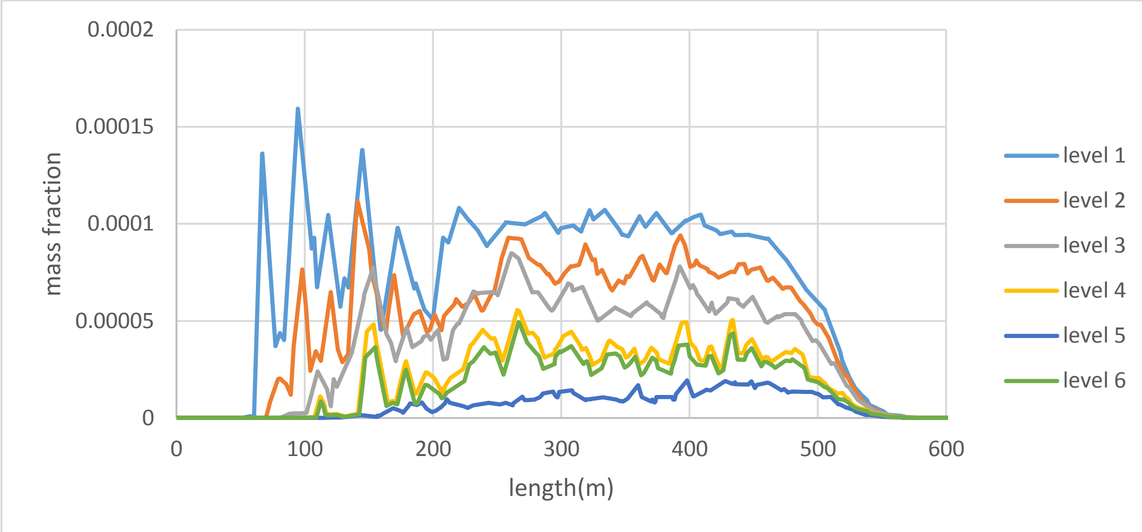

Figure 5.4.2 Nitrogen oxide dispersion

NOx gas had moved 550m downstream distance and the maximum mass fraction is 0.00015 on ground and the distance covered by the gas is more compared to the dispersion at wind velocity less than 7m/s.

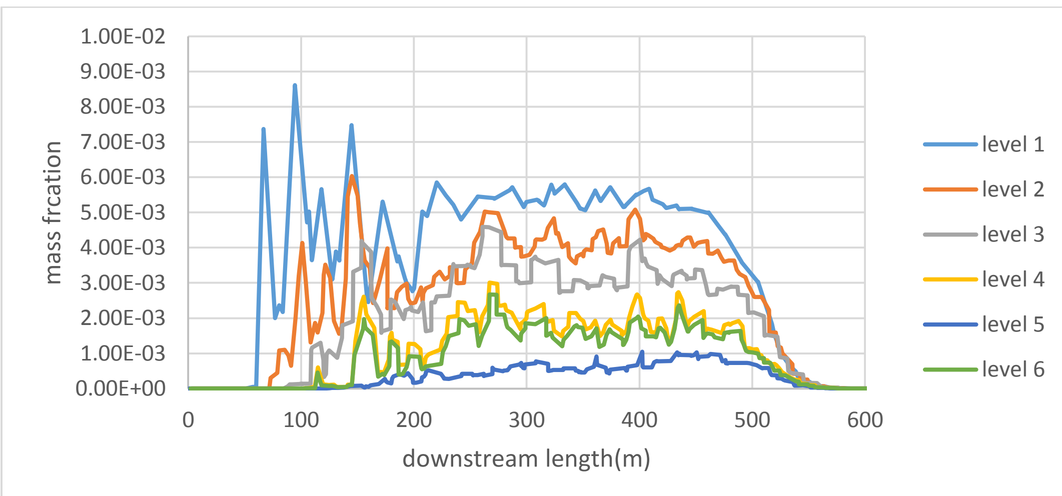

Figure 5.4.3 Carbon dioxide dispersion

CO_2gas had moved 550m downstream distance and the maximum mass fraction is 0.009 on ground at a distance of 100m and the concentration had been decreasing as it is moving downstream.

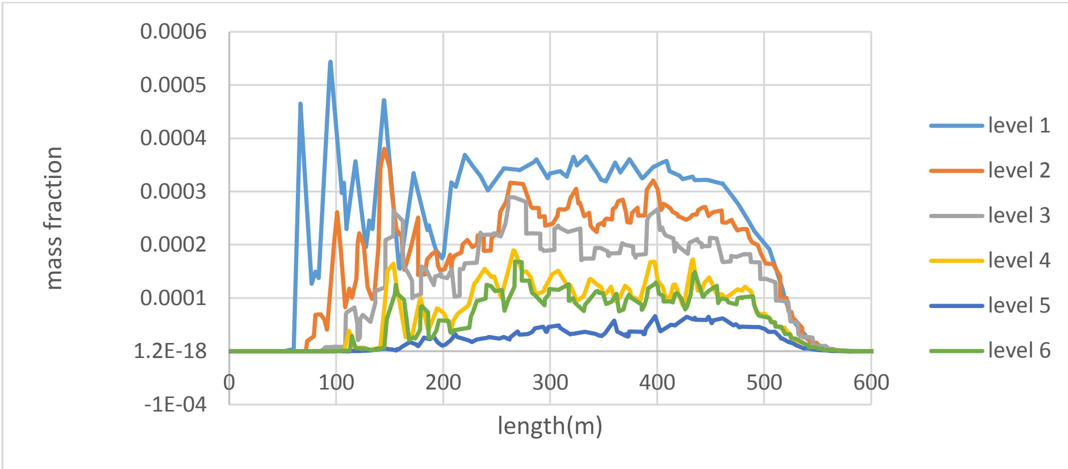

Figure 5.4.4 Carbon monoxide dispersion

CO gas had moved 550m downstream distance and the maximum mass fraction is 0.00055 on ground and the distance covered by the gas is more compared to the dispersion at wind velocity less than 7m/s. and the trend followed by the gas in all levels is almost the same.

5.5 Wind velocity at 9m/s

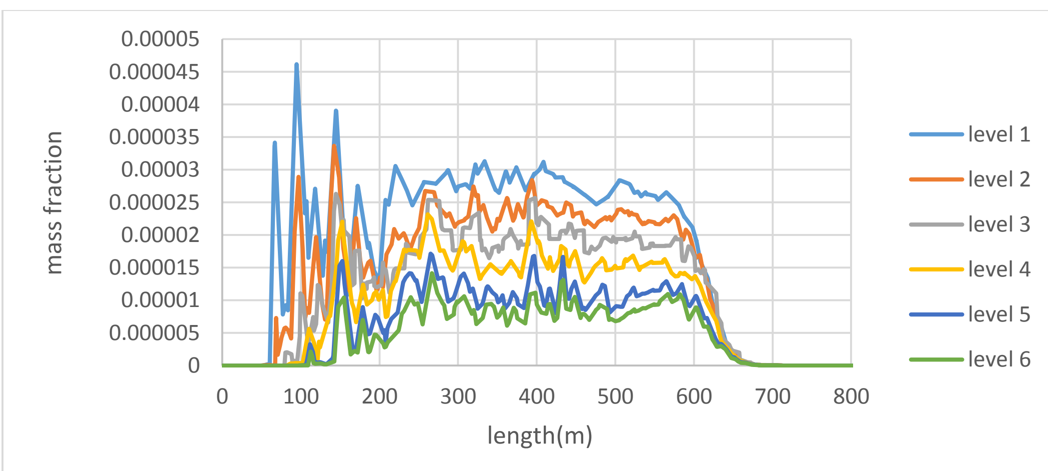

Figure 5.5.1 Sulphur dioxide dispersion

SO_2 gas is following a particular trend at all levels and the downstream length affected by the gas is almost 700m and the maximum mass fraction is 0.000045 on ground is at a distance of 100m.At 25m height the concentration of gas is not so less compared to ground level.

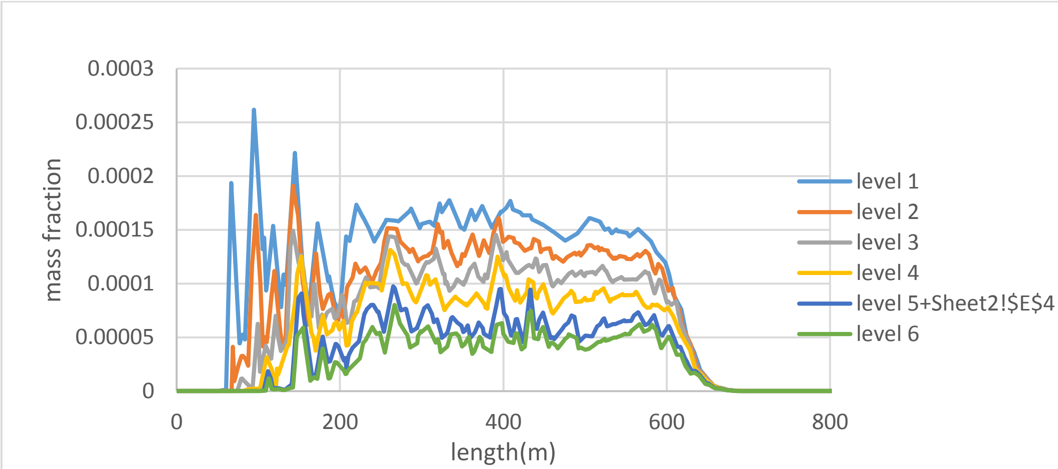

Figure 5.5.2 Nitrogen oxide dispersion

NOx gas is following a particular trend at all levels and the downstream length affected by the gas is 630m and the maximum mass fraction is 0.00025 on ground is at a distance of 95m.The concentration of the gas is decreasing as the height is increasing.

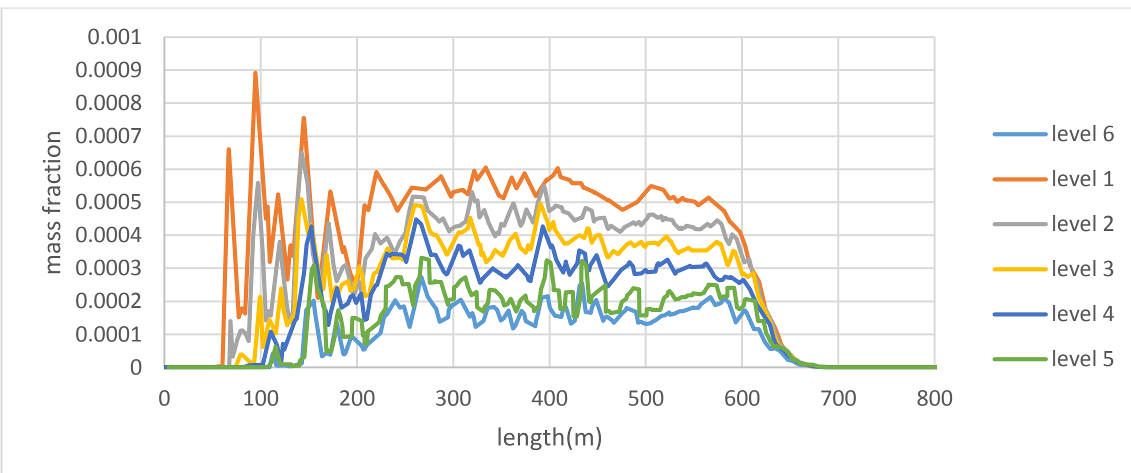

Figure 5.5.3 Carbon monoxide dispersion

CO gas is following a particular trend at all levels and the downstream length affected by the gas is nearly 690m and the maximum mass fraction is 0.0009 on ground is at a distance of 95m.

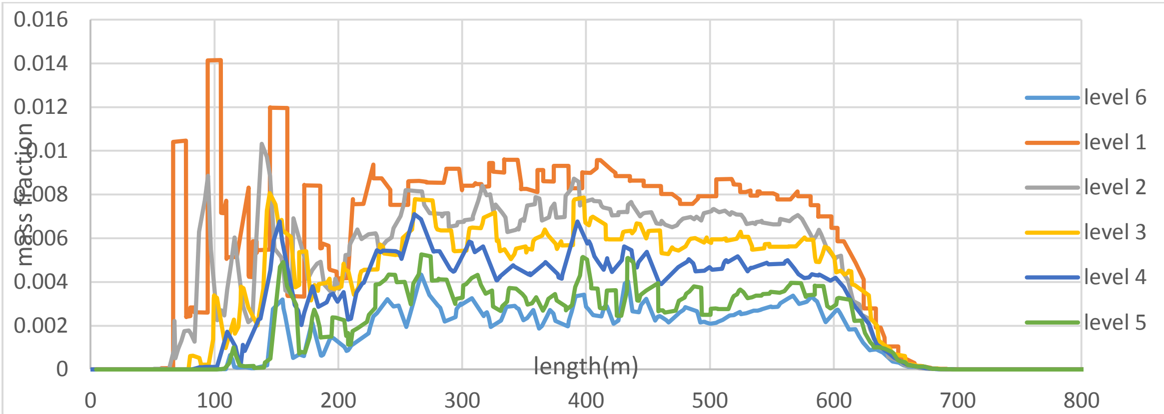

Figure 5.5.4 Carbon dioxide dispersion

CO gas is following a particular trend at all levels and the downstream length affected by the gas is 6900m and the maximum mass fraction is 0.014 on ground is at a distance of 100m.The dispersion to higher levels is increasing compared to previous cases where wind velocity is less than 9m/s.

5.6 Wind velocity at 11m/s

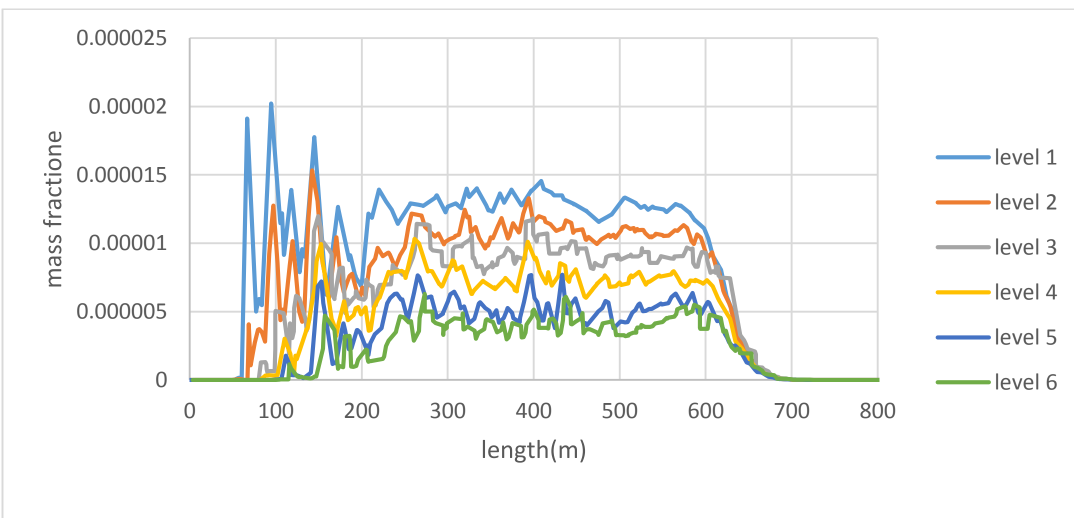

Figure 5.6.1 Sulphur dioxide dispersion

SO_2 gas is following a particular trend at all levels and the downstream length affected by gas is 7000m and the maximum mass fraction is 0.00002 on ground is at a distance of 98m.At 25m height also dispersion is quiet good with mass fraction 0.000005.

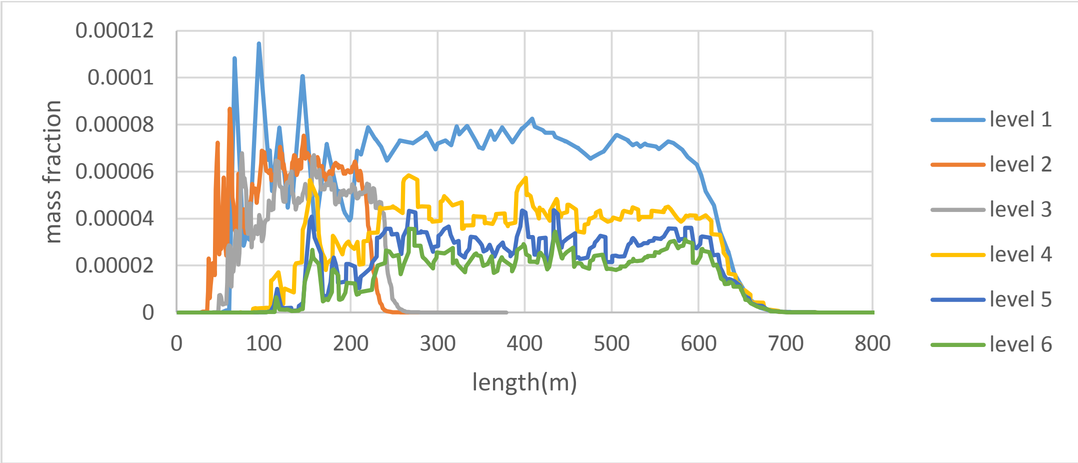

Figure 5.6.2 Nitrogen oxide dispersion

Downstream length affected by the gas is 7000m and the maximum mass fraction is 0.00012 on grounds is at a distance of 98m.As the concentration of gas is very low and as the velocity is more the gas at level 2 and level 3 had become zero at a distance of 300m.

5.7 Wind velocity at 13 m/s

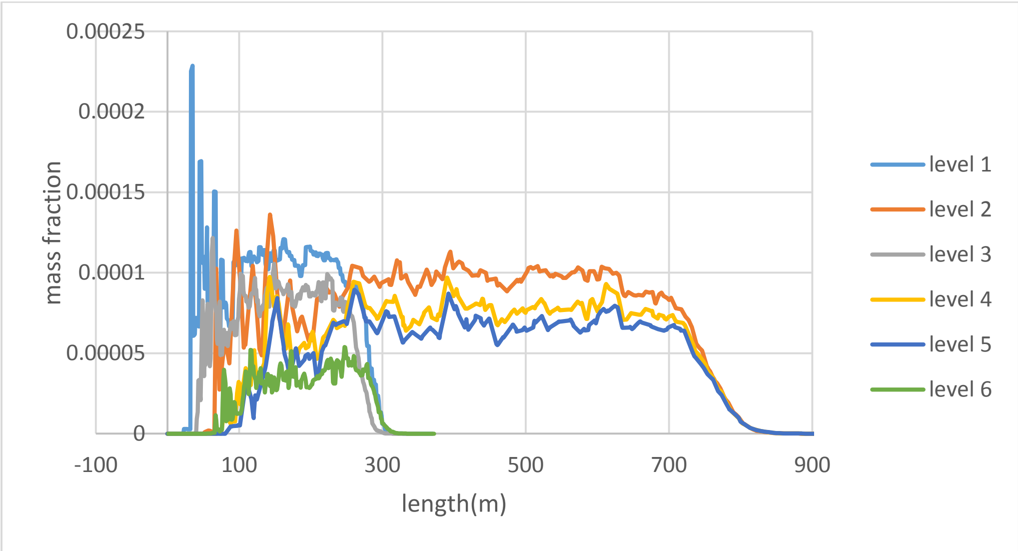

Figure 5.7.1 Carbon monoxide dispersion

The downstream length affected by the gas is nearly 900m and the maximum mass fraction is 0.00023 on ground.

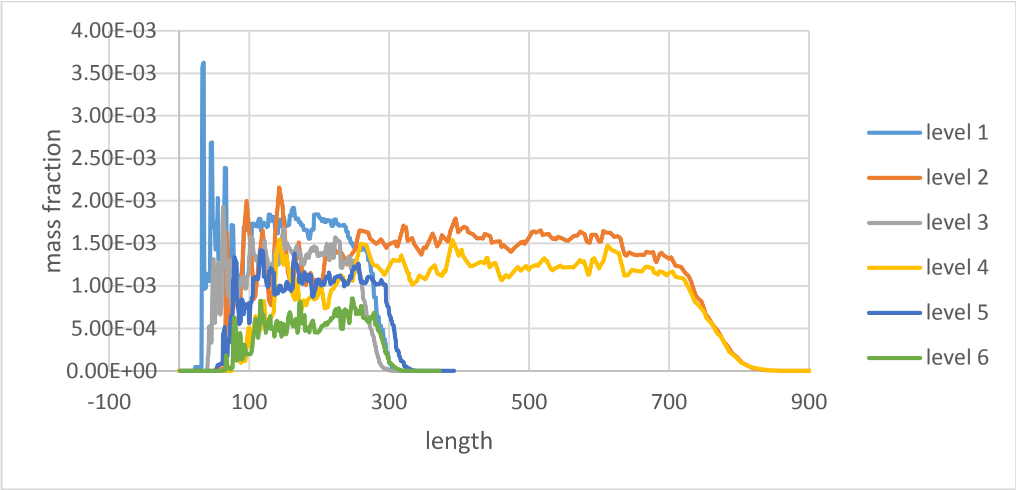

Figure 5.7.2 Carbon dioxide dispersion

The downstream length affected by the gas is nearly 900m and the maximum mass fraction is 0.0035 on ground and levels which have less concentration initially have settled to ground at a distance of 300m.

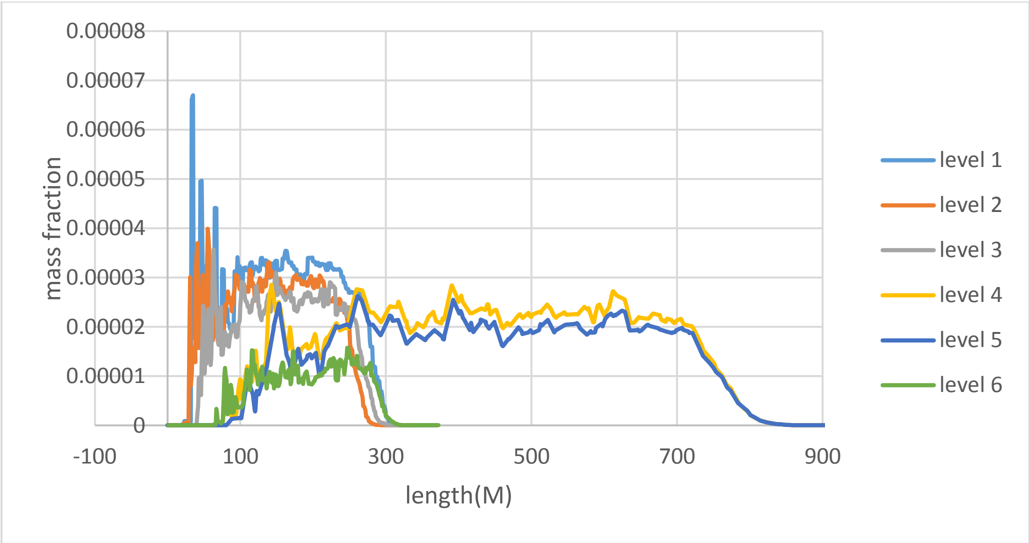

Figure 5.7.3 Nitrogen oxide dispersion

The downstream length affected by the gas is nearly 900m and the maximum mass fraction is 0.000065 on ground and the concentration has been decreasing as the height is increasing.

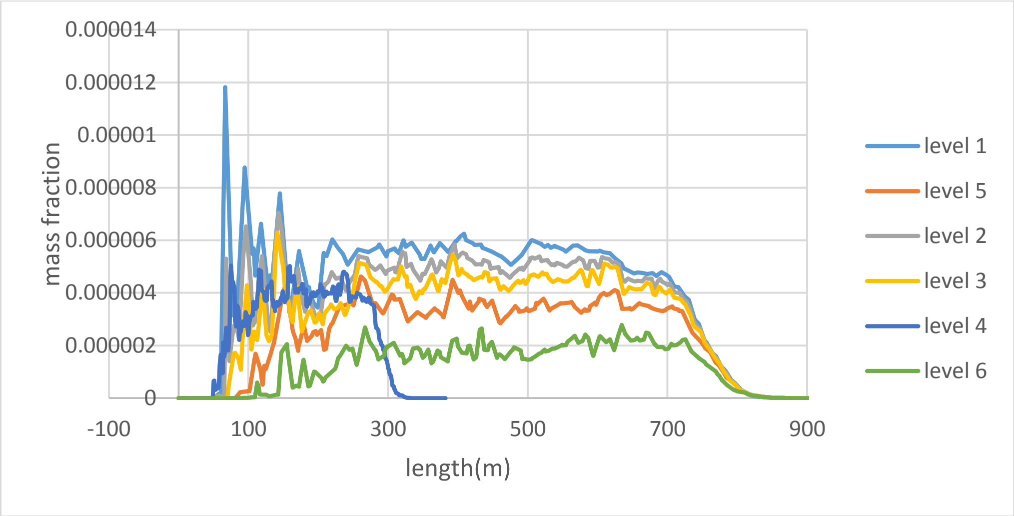

Figure 5.7.4 Sulphur dioxide dispersion

The gas is following almost the same trend except at level 4 and the length covered by gas is almost 900m.

5.8 Wind velocity at 15m/s

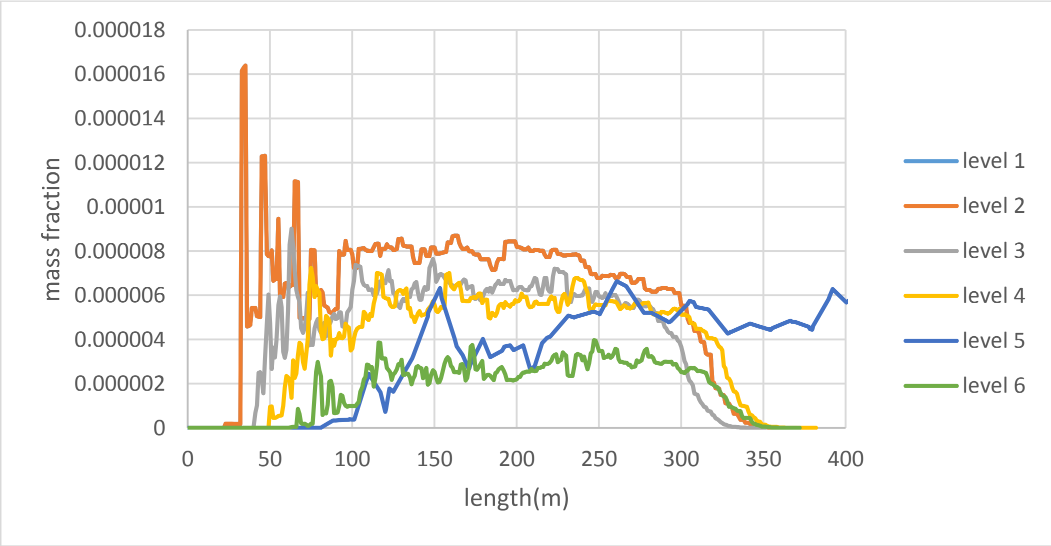

Figure 5.8.1 Sulphur dioxide dispersion

The downstream length affected by the gas is 900m and the maximum mass fraction is 0.0016 on ground. At 25m height the concentration of gas is nearly 0.000002.

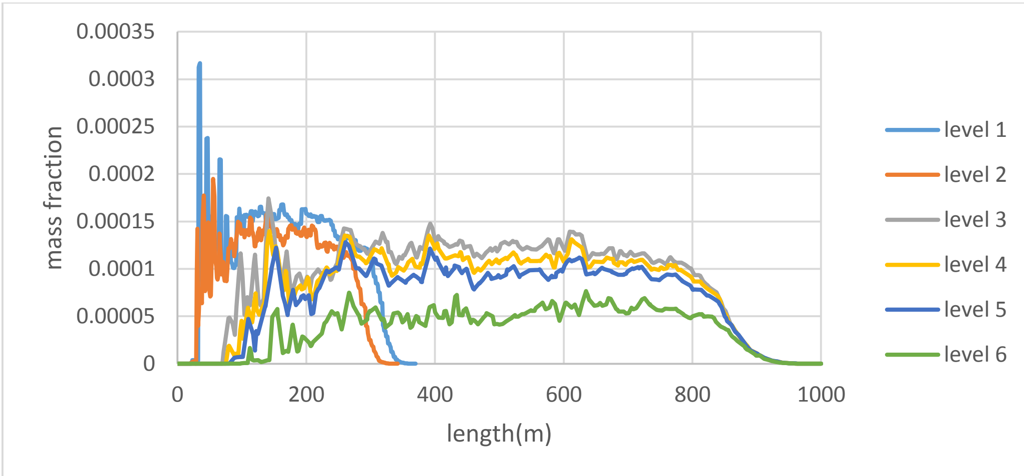

Figure 5.8.2 Carbon dioxide dispersion

The downstream length affected by the gas is greater than 900m, and the maximum mass fraction is 0.0003.The concentration of the gas is decreasing as the height increases.

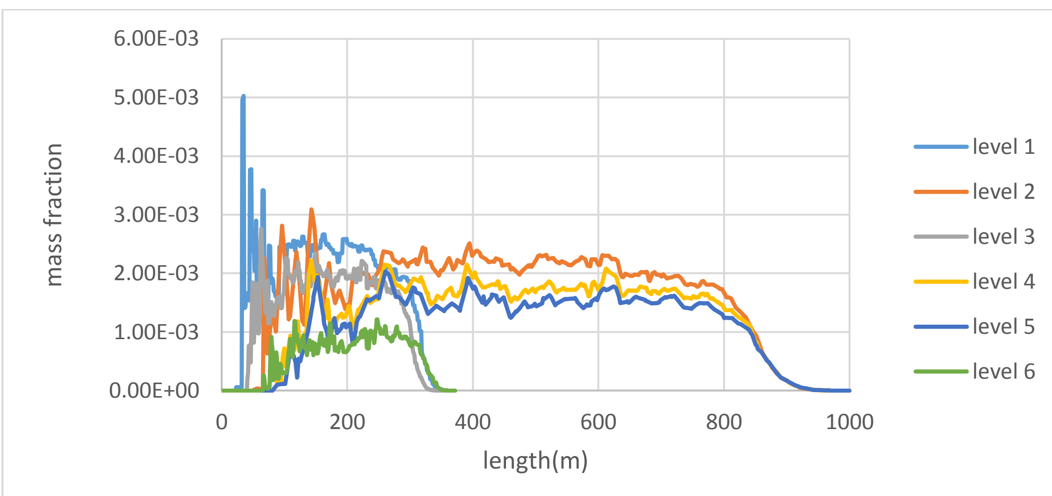

Figure 5.8.3 Carbon dioxide dispersion

The downstream length affected by the gas is greater than 900m and the maximum mass fraction is 0.0005 on ground .At 25m height the concentration of gas has become zero at a distance nearly 400m.

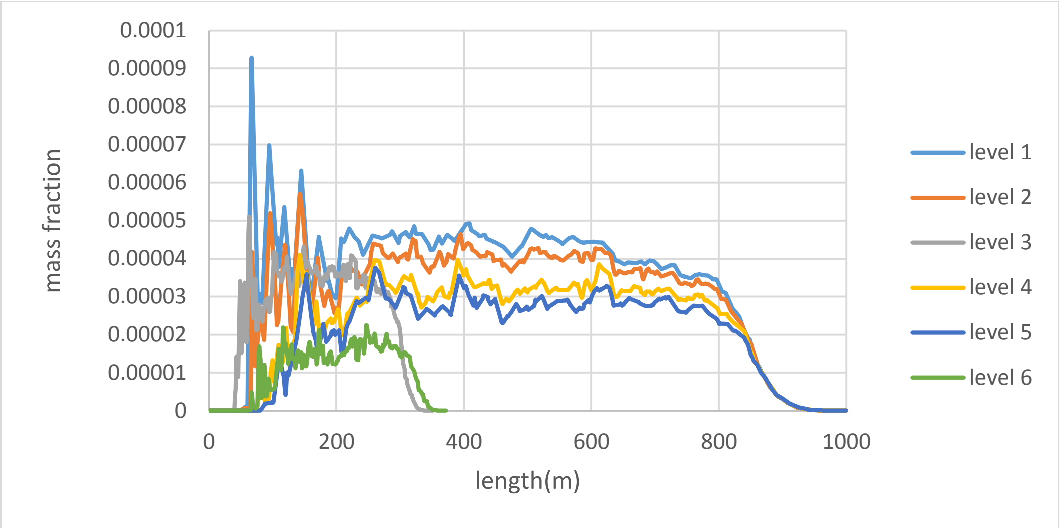

Figure 5.8.4 Nitrogen oxide dispersion

The gas affects downstream length greater than 900m and the concentration is decreasing down the downstream length.

5.9 Wind velocity at 17m/s

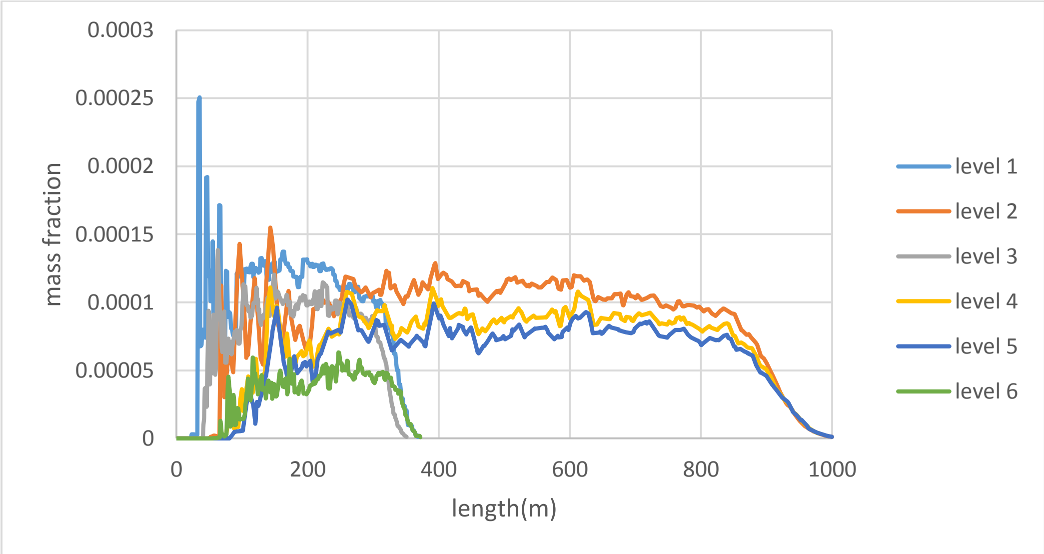

Figure 5.9.1 Carbon monoxide dispersion

The downstream length covered by the gas is 1000m, as the initial concentration is less the concentration at the last level is less and it is settling on ground at a distance of 400m.

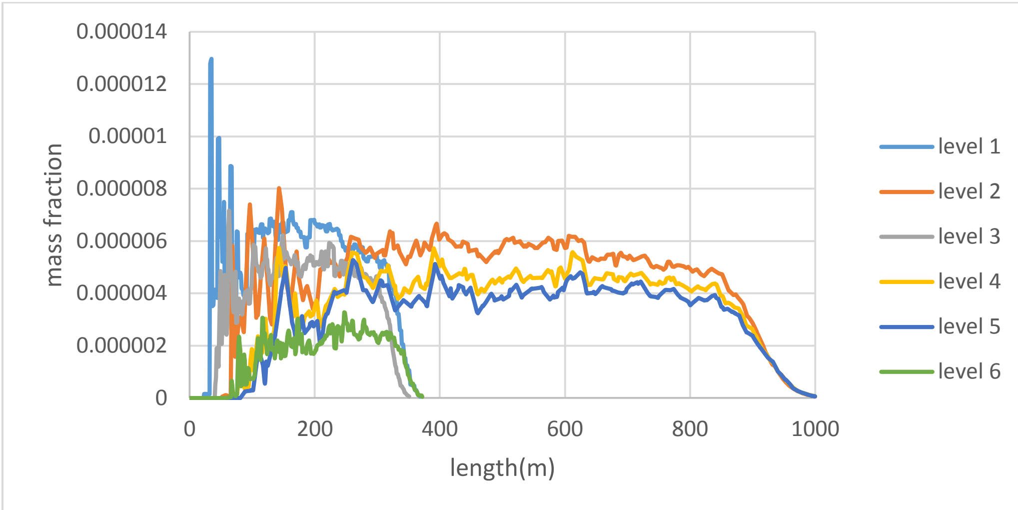

Figure 5.9.2 Sulphur dioxide dispersion

The downstream length covered by the gas is 1000m and as the height is increasing the concentration has been decreasing.

5.10 Wind velocity at 19m/s

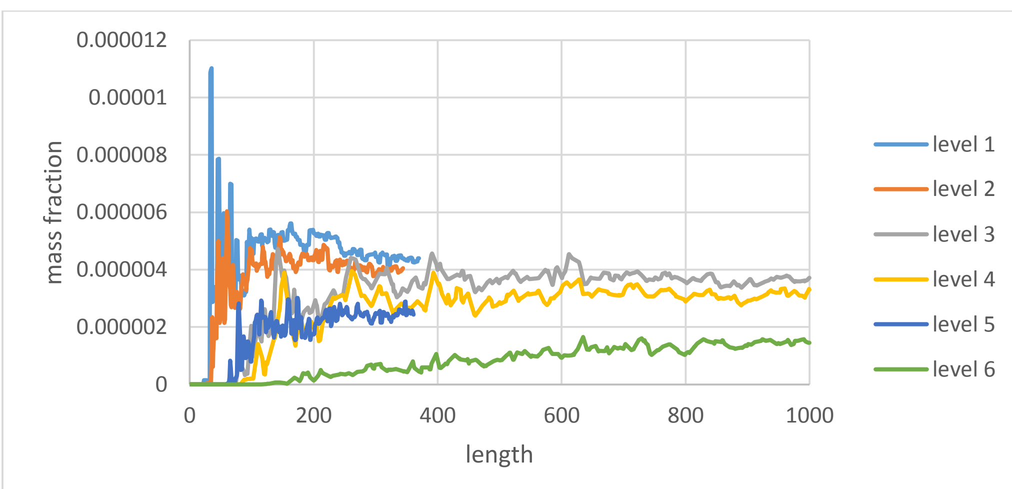

Figure 5.10.1 Sulphur dioxide dispersion

The gas is moving a downstream length greater than 1000m and at this velocity it is not getting settled on ground and the maximum concentration is on ground and the value is nearly 0.000011.

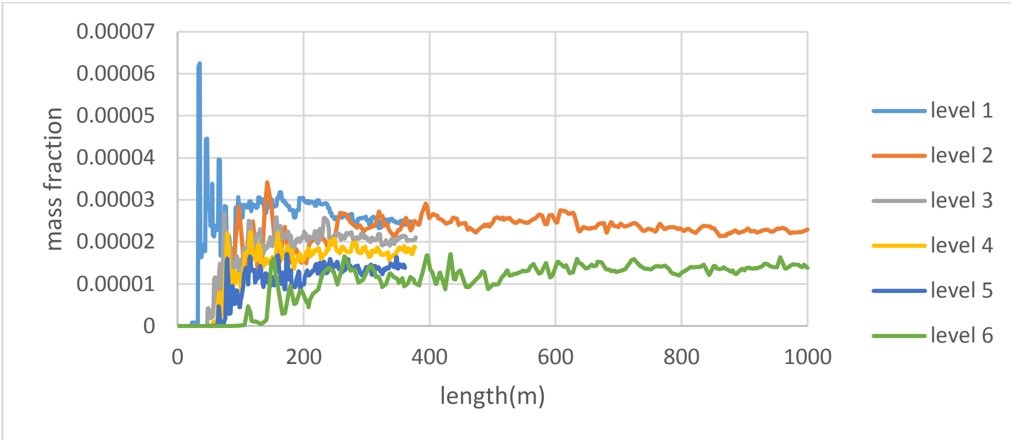

Figure 5.10.2 Nitrogen oxide dispersion

The gas is moving a downstream length greater than 1000m and at this velocity it is not getting settled on ground and the maximum concentration is on ground and the value is nearly 0.00006.

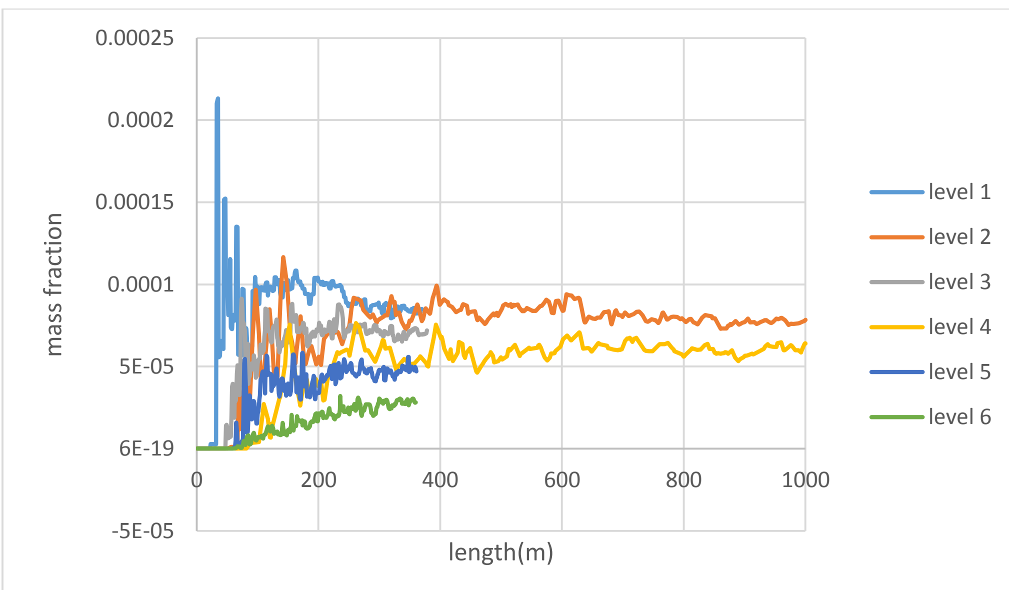

Figure 5.10.3 Carbon monoxide dispersion

The gas is moving a downstream length greater than 1000m and at this velocity gas is dispersed throughout instead of settling on ground.

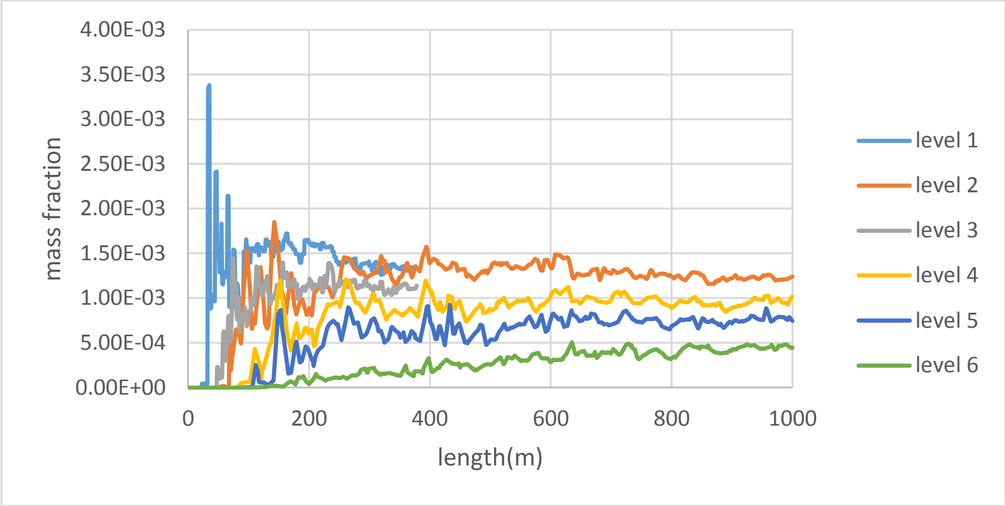

Figure 5.10.4 Carbon dioxide dispersion

The gas is moving a downstream length greater than 1000m and as Carbon dioxide concentration is more, gas present at different levels is going beyond 1000m which is not the case for NOx ,CO.

At 1m/s wind velocity, gases had settled on ground at a distance of 150 m. At all levels, gases followed a particular trend. As the wind velocity is increased to 3m/s, 5m/s, gases had settled at a distance of 250 m, 350 m following similar trend at different levels. Level 6 which is at the maximum height compared to others has a very low concentration of gases compared to all other levels. At wind velocity 6m/s, 7m/s gases had settled at a distance of 550m, 650m.As the height from the ground level is increasing, the concentration of gases is decreasing. At wind velocity 9m/s, 11m/s gases are covering downstream distance of nearly 800m. As the wind velocity is increased above 13m/s, gases crossed a downstream distance of 900m.Gases which are near to ground is settling vastly compare to gases which are at a height more than 10m .At the max wind velocity of 19m/s gases had crossed 1000m.As carbon dioxide concentration is more than Sulphur dioxide, nitrogen oxide, carbon monoxide, this gas at 1000m/s wind velocity had crossed 1000m downstream length at different levels whereas for other gases they have been dispersed and didn't settle .As the wind velocity is increased gas concentration near to the ground has been decreasing and as the height is increasing the concentration has been increasing. As the wind velocity is increased from 1m/s to 9m/s particular gas at different levels have been following the same trend whereas as the wind velocity is increased from 13m/s to 19m/s there is no such particular trend and the gas at different levels started settling randomly. The maximum mass fraction for all the gases at wind velocities less than 9m/s is at the ground level and at a distance of 90-100m roughly. As the Wind velocity has been increasing the concentration of the gases at the level 6 has been increasing.

CONCLUSION:

As the velocity is increased from 1m/s to 19m/s it is clear that the gases released from combustion of coal tar are covering more distance in down wind direction. The maximum concentrations of gases on ground level are mostly observed at a distance less than 100m. The concentration of the gases at a particular wind velocity has been decreasing as the height increases. As the velocity is increased from 1m/s to 9 m/s, concentration profiles are following a particular path whereas, as the velocity is increased beyond 11 m/s, ground level gases and gases at level 1 concentration are becoming zero as they are travelling half the downstream distance travelled by other gases at the same velocity. As the velocity is increased the concentration of gas settling on ground has decreased.

6. REFERENCES

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